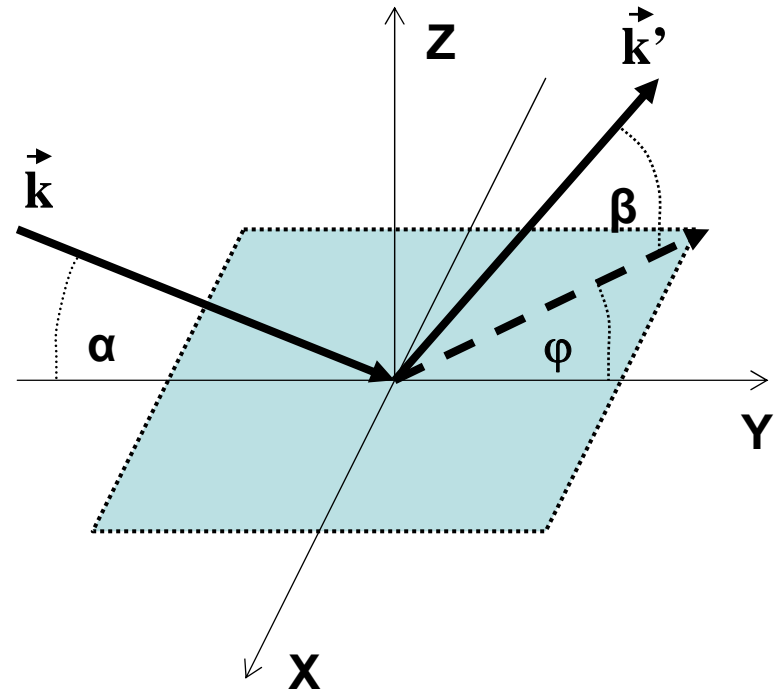


# Liquid Surface scattering geometry and reciprocal space

Scheme of surface scattering geometry shown on the right. The liquid surface is in the x-y plane, with the normal z pointing upwards. The wave vector  $\mathbf{k}$  of the incoming beam is in the y-z plane, making a (grazing) angle  $\alpha$  with the surface. The wave vector  $\mathbf{k}'$  of the scattered radiation is at angle  $\beta$  to the surface and, in general, its projection on the surface makes an angle  $\varphi$  (the in-plane angle) with the y-axis.

The magnitude of the wave vectors is related to the wavelength  $\lambda$  through

$$|\mathbf{k}| = |\mathbf{k}'| = k = 2\pi/\lambda$$



# Wave vector (momentum) exchange – q-vector

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Elastic wave scattering ↔ Diffraction

The amplitude of diffracted radiation is

$$A \propto \sum_j R_j \exp(i\mathbf{q} \cdot \mathbf{r}_j)$$

Where  $R_j$  is a local “response function” at position  $\mathbf{r}_j$  and  $\mathbf{q}$  is the radiative momentum exchange

$$\mathbf{q} = \mathbf{k}' - \mathbf{k}$$

The physics of surface scattering consists of determining (experimentally or theoretically) the amplitude of the scattered radiation as a function of  $\mathbf{q}$ .

Even though  $\mathbf{q}$  is a 3D vector, the components are not independent, being related by

$$|\mathbf{k}'| = |\mathbf{k}| \quad \leftrightarrow \quad |\mathbf{k} + \mathbf{q}| = |\mathbf{k}| \quad \leftrightarrow \quad |\mathbf{q}|^2 + 2\mathbf{k} \cdot \mathbf{q} = 0$$

Therefore, the scattering process can be analyzed using two scalar parameters.

# Geometry $\leftrightarrow$ q-vector

A convenient choice of parameters is:

1.  $q_z$  - The z (normal) component of  $\mathbf{q}$ .
2.  $q_{xy}$  - The absolute value of the xy (in-plane) projection of  $\mathbf{q}$ .

Note that while  $q_z$  is a vector component,  $q_{xy}$ , in general, is not.

Expressing  $\mathbf{k}$  and  $\mathbf{k}'$  explicitly in terms of angles as

$$\mathbf{k} = k(0, \cos \alpha, -\sin \alpha)$$

$$\mathbf{k}' = k(-\cos \beta \sin \varphi, \cos \beta \cos \varphi, \sin \beta)$$

And using the definition of  $\mathbf{q}$ , we get

$$q_z = k(\sin \alpha + \sin \beta)$$

$$q_{xy} = k\sqrt{\cos^2 \alpha - 2 \cos \alpha \cos \beta \cos \varphi + \cos^2 \beta}$$

For calculations it is better to use

$$q_z = 2k \sin \frac{\beta + \alpha}{2} \cos \frac{\beta - \alpha}{2}$$

$$q_{xy} = 2k \sqrt{\sin^2 \frac{\beta + \alpha}{2} \sin^2 \frac{\beta - \alpha}{2} + \cos \alpha \cos \beta \sin^2 \frac{\varphi}{2}}$$

# Some practical issues

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Typically measurements are performed scanning one of the angles while keeping the other ones fixed, or (in the case of reflectivity measurement) scanning two angles ( $\alpha$  and  $\beta$ ) jointly while keeping the third ( $\varphi$ ) fixed. Then results are displayed and analyzed as a function of  $q_z$  and/or  $q_{xy}$ .

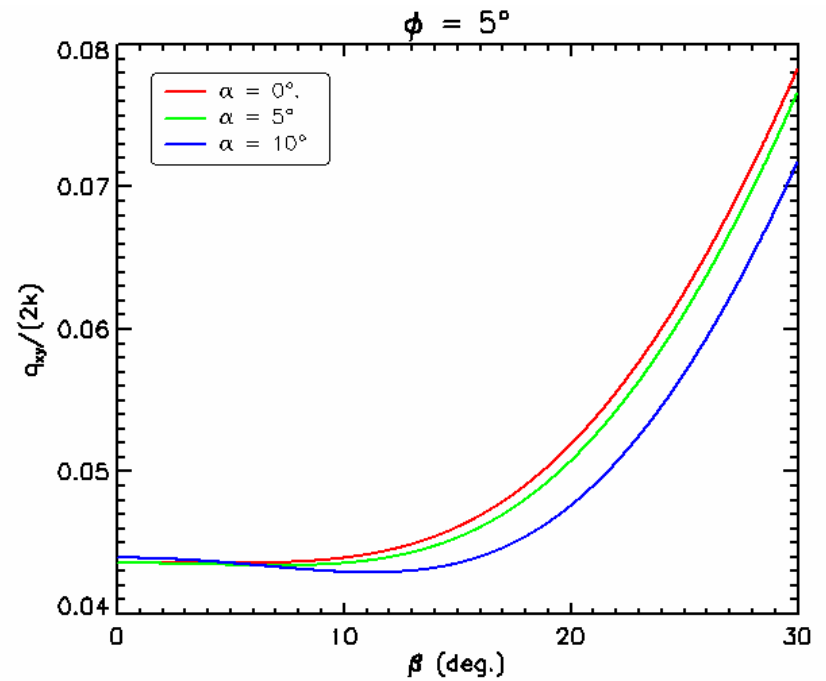
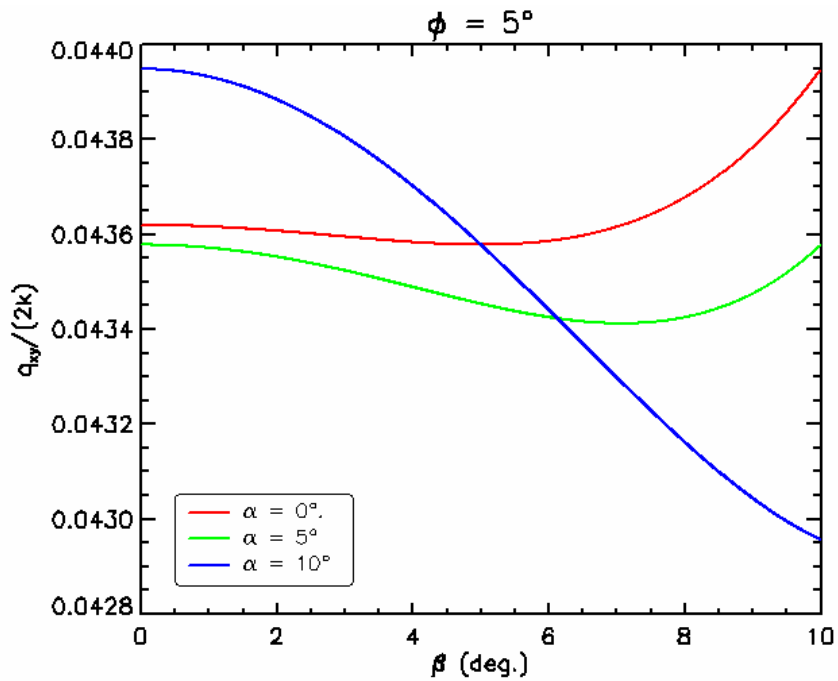
Roughly speaking, we've the equivalence:

$$\begin{aligned}\alpha, \beta &\leftrightarrow q_z \\ \varphi &\leftrightarrow q_{xy}\end{aligned}$$

Strictly speaking, though, the above is only half true. In detail:

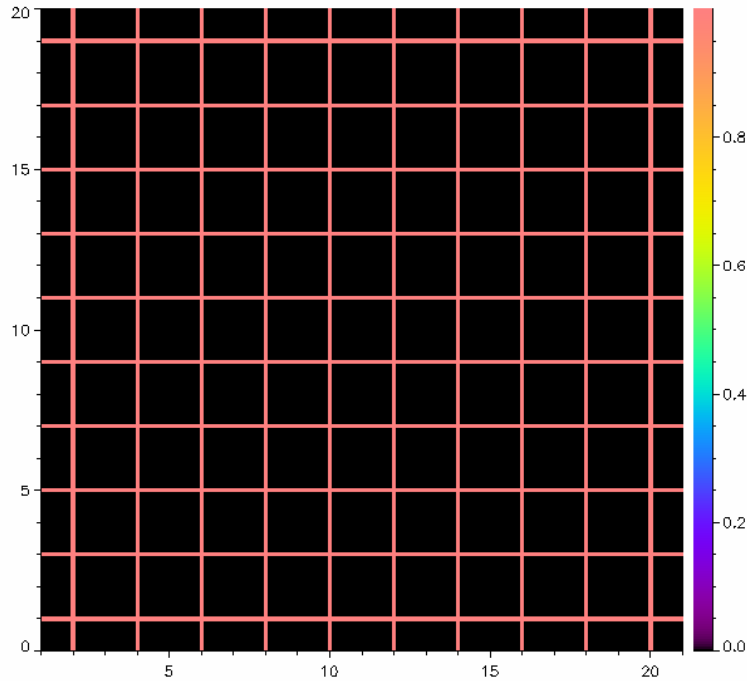
- Varying  $\varphi$  while keeping  $\alpha$  and  $\beta$  fixed is, indeed, equivalent to varying  $q_{xy}$  while keeping  $q_z$  fixed.
- On the other hand, keeping  $\varphi$  fixed and varying  $\alpha$ ,  $\beta$  or both, does, in general result in varying **both**  $q_z$  and  $q_{xy}$ , though as long as both  $\alpha$  and  $\beta$  are small enough, the variation of  $q_{xy}$  may be small enough to be neglected. The only case where  $q_z$  alone changes is when  $\varphi = 0$  and  $\alpha$ ,  $\beta$  are varied jointly so that  $\alpha = \beta$ . This is the case of *reflectivity* measurement.

# $q_{xy}$ variation with constant $\varphi$

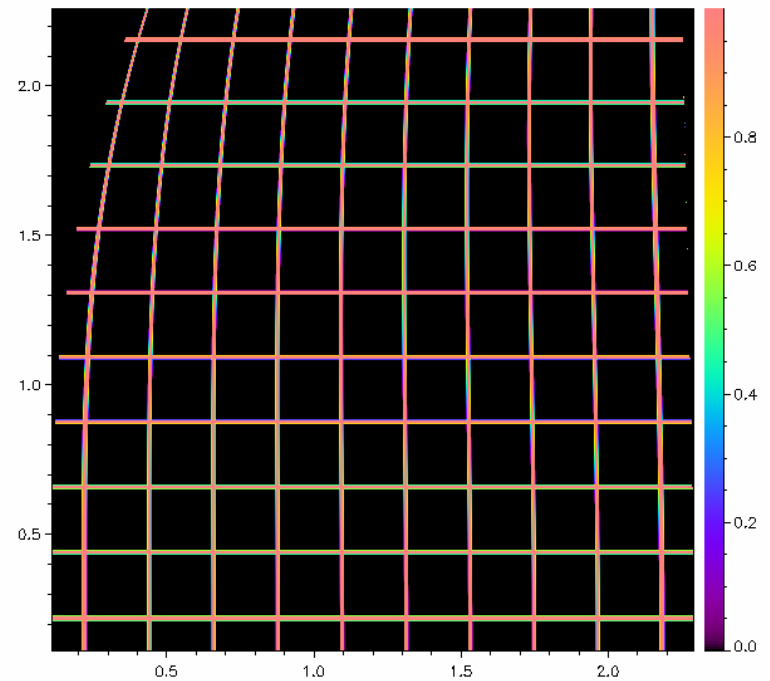


# More on $q_{xy}$ variation

Angle grid ( $\varphi$ - $\beta$ )



Corresponding  $q_{xy} - q_z$  grid, with  $\alpha = 2^\circ$  and wavelength of  $1\text{\AA}$

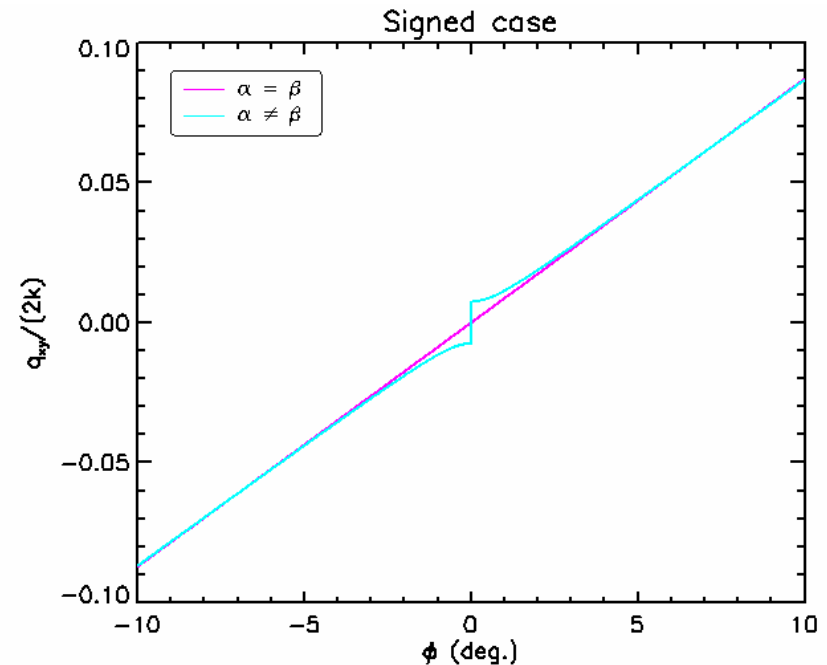
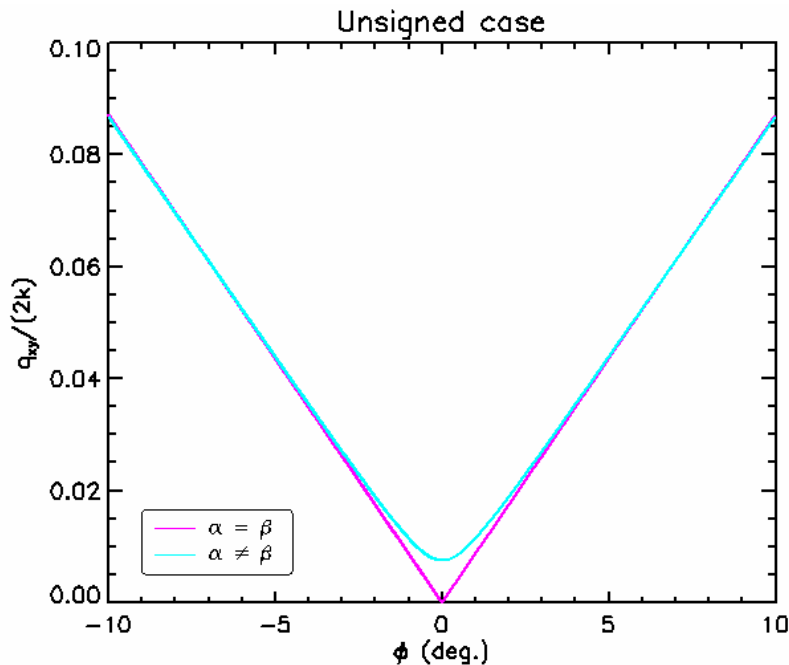


# Problems around $\varphi = 0$

The fact that the deformation is especially pronounced for small values of  $\varphi$  is not accidental. It stems from the fact that the transformation from angles to  $q_{xy}$  is ill conditioned at  $\varphi = 0$ . In fact, it is double valued there, which is **not good**.

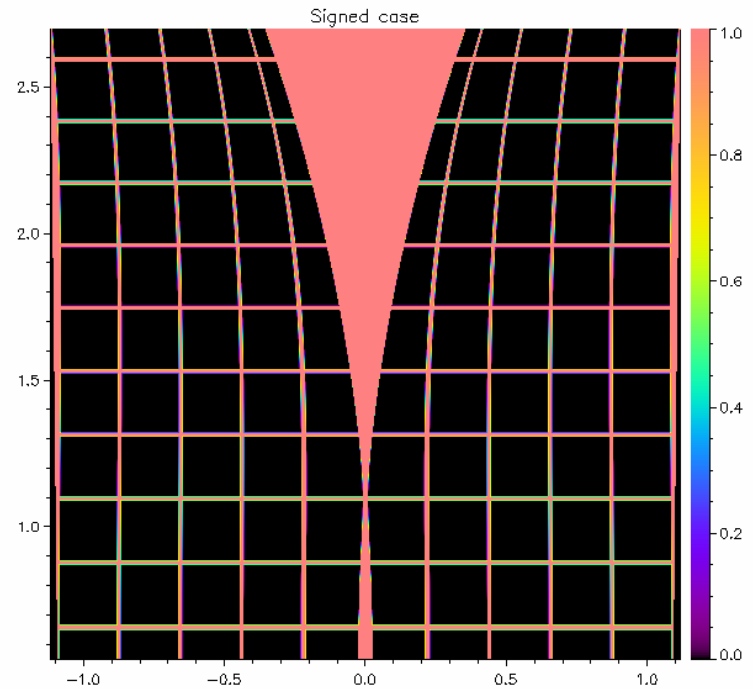
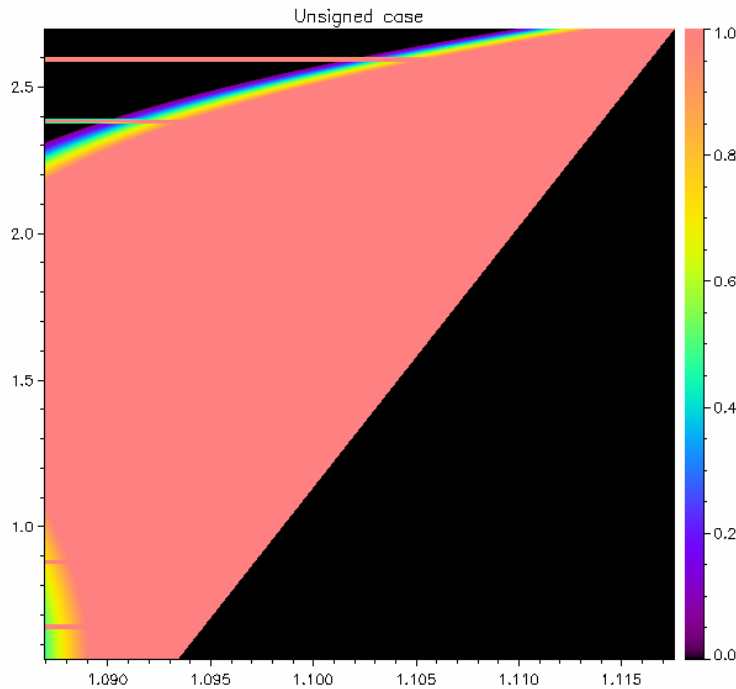
The problem can seemingly be fixed by using a “signed” value of  $q_{xy}$  multiplied by  $\text{sign}(\varphi)$ . This eliminates the double-valueness but introduces, instead, a discontinuity, except when  $\alpha = \beta$ .

Thus, in general, the region around  $\varphi = 0$  should be treated with great care.



# More about problems

Transforming 2D data around  $\varphi = 0$ . Unsigned transformation creates a mess. Signed one behaves better, but at the price of a “hole” opening in the data.



# Steering crystal alignment problem

Beyond its relevance to the physics of surface scattering, geometry is of great value at the technical level of precision alignment.

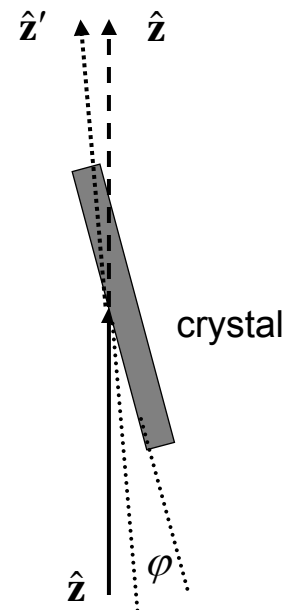
As an example, we may consider the directional alignment of a steering crystal to the beam.

Drawing on the right: top view of steering crystal as mounted in the 3-circle. Beam direction is  $\mathbf{z}$  and the direction of the “along the beam” axis of the 3-circle is  $\mathbf{z}'$ .

For the purpose of measurement we:

1. Rotate the crystal by an angle  $\varphi$  around the vertical axis, to obtain a Bragg reflection (for  $\mathbf{z} = \mathbf{z}'$ ,  $\varphi = \theta_B$ ).
2. Rotate the crystal around the  $\mathbf{z}'$  axis, by an angle  $\chi$ , to steer the beam downward. For  $\mathbf{z} = \mathbf{z}'$  such rotation does not change the beam-crystal angle.

Obviously, proper alignment, here, means  $\mathbf{z} = \mathbf{z}'$ . When this is not so, the beam will get lost upon  $\chi$  – rotation.



## ...And solution

As is often the case, the problem carries with it its own solution. Since a deviation of  $\mathbf{z}$  from  $\mathbf{z}'$  results in  $\phi$  varying with  $\chi$ , then this variation can be used to find the extent of the deviation and correct for it. In detail, denoting the horizontal and vertical angular deviations of  $\mathbf{z}'$  by  $\varepsilon_x$  and  $\varepsilon_y$  and applying some geometry (and algebra) we get, for the angle  $\phi$  corresponding to reflection maximum, the result (first order)

$$\phi \approx \theta_B - \varepsilon_x \cos \chi + \varepsilon_y \sin \chi$$

So, we perform three consecutive measurements of  $\phi$ , at  $\chi$  values of 0,  $-\chi_A$  and  $\chi_A$  and get the equations:

$$\phi_0 = \theta_B - \varepsilon_x$$

$$\phi_- = \theta_B - \varepsilon_x \cos \chi_A - \varepsilon_y \sin \chi_A$$

$$\phi_+ = \theta_B - \varepsilon_x \cos \chi_A + \varepsilon_y \sin \chi_A$$

which can be solved to yield

$$\varepsilon_x = \frac{\phi_+ + \phi_- - 2\phi_0}{2(1 - \cos \chi_A)} = \frac{\phi_+ + \phi_- - 2\phi_0}{4 \sin^2 \frac{\chi_A}{2}}$$

$$\varepsilon_y = \frac{\phi_+ - \phi_-}{2 \sin \chi_A} = \frac{\phi_+ - \phi_-}{4 \sin \frac{\chi_A}{2} \cos \frac{\chi_A}{2}}$$